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MODIFICATIONS AND ALTERNATIVES TO THE CUBIC INTERPOLATION PROCESS FOR ONE-DIMENSIONAL SEARCH

by

A. MIELE, F. BONARDO, and S. GONZALEZ

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

In this paper, the numerical solution of the problem of minimizing a unimodal function $f(\alpha)$ is considered, where α is a scalar. Two modifications of the cubic interpolation process are presented, so as to improve the robustness of the method and force the process to converge in a reasonable number of (OVER)

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19. KEY WORDS (Continued)

process, mathematical programming, interval of interpolation, numerical analysis, numerical methods, computing methods, computing techniques.

20. ABSTRACT (Continued)

iterations, even in pathological cases. Modification M1 includes the nonoptional bisection of the interval of interpolation at each iteration of the process. Modification M2 includes the optional bisection of the interval of interpolation: this depends on whether the slopes $f_\alpha(\hat{\alpha}_0)$ and $f_\alpha(\alpha_0)$ at the terminal points $\hat{\alpha}_0$ and α_0 of two consecutive iterations have the same sign or opposite sign.

An alternative to the cubic interpolation process is also presented. This is a Lagrange interpolation scheme in which the quadratic approximation to the derivative of the function is cor[illegible]d. The coefficients of the quadratic are determined from the values of the slope at three

alpha sub 1 alpha sub 3 alpha sub 1

points: α_1, α_2, and $\alpha_3 = (\alpha_1+\alpha_2)/2$, where α_1 and α_2 are the endpoints

alpha sub 2

of the interval of interpolation. The proposed alternative is investigated in two versions, Version A1 and Version A2. They differ in the way in which the next interval of interpolation is chosen; for Version A1, the choice depends on the sign of the slope $f_\alpha(\alpha_0)$; for Version A2, the choice depends on the signs of the slopes $f_\alpha(\alpha_0)$ and $f_\alpha(\alpha_3)$.

Twenty-nine numerical examples are presented. The numerical results show that both modifications of the cubic interpolation process improve the robustness of the process. They also show the promising characteristics of Version A2 of the proposed alternative. Therefore, the one-dimensional search schemes described here have potential interest for those minimization algorithms which depend critically on the precise selection of the stepsize, namely, conjugate gradient methods.

Modifications and Alternatives to the Cubic Interpolation Process for One-Dimensional Search[1]

by

A. MIELE[2], F. BONARDO[3], and S. GONZALEZ[4]

Abstract. In this paper, the numerical solution of the problem of minimizing a unimodal function $f(\alpha)$ is considered, where α is a scalar. Two modifications of the cubic interpolation process are presented, so as to improve the robustness of the method and force the process to converge in a reasonable number of iterations, even in pathological cases. Modification M1 includes the nonoptional bisection of the interval of interpolation at each iteration of the process. Modification M2 includes the optional bisection of the interval of interpolation: this depends on whether the slopes $f_\alpha(\hat{\alpha}_o)$ and $f_\alpha(\alpha_o)$ at the terminal points $\hat{\alpha}_o$ and α_o of

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two consecutive iterations have the same sign or opposite sign.

An alternative to the cubic interpolation process is also presented. This is a Lagrange interpolation scheme in which the quadratic approximation to the derivative of the function is considered. The coefficients of the quadratic are determined from the values of the slope at three points: α_1 , α_2 , and $\alpha_3 = (\alpha_1+\alpha_2)/2$, where α_1 and α_2 are the end-points of the interval of interpolation. The proposed alternative is investigated in two versions, Version A1 and Version A2. They differ in the way in which the next interval of interpolation is chosen; for Version A1, the choice depends on the sign of the slope $f_\alpha(\alpha_o)$; for Version A2, the choice depends on the signs of the slopes $f_\alpha(\alpha_o)$ and $f_\alpha(\alpha_3)$.

Twenty-nine numerical examples are presented. The numerical results show that both modifications of the cubic interpolation process improve the robustness of the process. They also show the promising characteristics of Version A2 of the proposed alternative. Therefore, the one-dimensional search schemes described here have potential interest for those minimization algorithms which depend critically on the precise selection of the stepsize, namely, conjugate gradient methods.

Key Words. One-dimensional search, cubic interpolation process, quadratic interpolation process, Lagrange interpolation scheme, modifications of the cubic interpolation process, alternatives to the cubic interpolation process, bisection process, mathematical programming, interval of interpolation, numerical analysis, numerical methods, computing methods, computing techniques.

1. Introduction

Many algorithms for mathematical programming problems consist of two parts: the computation of the search direction and the computation of the stepsize along the search direction chosen. The computation of the stepsize is done by means of one-dimensional search schemes, whose nature (i.e., approximate or precise) must be tailored to the characteristics of the algorithm under consideration.

For algorithms of the pointwise type (i.e., ordinary gradient method and quasilinearization method), approximate search schemes can be employed. On the other hand, for algorithms of the cyclic type (i.e., conjugate gradient methods and variable-metric methods), precise search schemes are desirable (see, for example, Refs. 1-3).

Among the search schemes available, one of the most widely used is the cubic interpolation process (see Ref. 4). In the standard process (a Hermite process), the function $f(\alpha)$ is approximated by a cubic, and the coefficients of the cubic are determined from the values of the ordinate $f(\alpha)$ and the slope $f_\alpha(\alpha)$ at two points α_1 and α_2 , chosen so that $f_\alpha(\alpha_1) < 0$ and $f_\alpha(\alpha_2) > 0$. In an alternative process (Ref. 5), the coefficients of the cubic are determined from the values of the ordinate $f(\alpha)$ at four points.

Another widely used search scheme is the quadratic interpolation process (see Refs. 6-7). In the standard process, the function $f(\alpha)$ is approximated by a quadratic, and the coefficients of the quadratic are determined from the values of the ordinate $f(\alpha)$ at three points. In an alternative process (Ref. 8), the coefficients of the quadratic are determined from the values of the ordinate $f(\alpha)$ at two points and the slope $f_\alpha(\alpha)$ at one point.

In this paper, we consider the Hermite cubic interpolation process, and we present some modifications of the process, designed to improve the robustness of the method and force the process to converge in a reasonable number of iterations, even in pathological cases. The function $f(\alpha)$ is approximated in the same way as in the standard process, but a new feature is added: a bisection of the interval of interpolation, which is done, either nonoptionally or optionally, in accordance with certain rules described in Section 3.

Next, an alternative to the cubic interpolation process is presented in Section 4. This is a Lagrange interpolation scheme, in which a quadratic approximation to the derivative of the function is considered. The coefficients of the quadratic polynomial are determined from the values of the slope $f_\alpha(\alpha)$ at three points: α_1, α_2, α_3 . The points α_1 and α_2 are such that $f_\alpha(\alpha_1) < 0$ and $f_\alpha(\alpha_2) > 0$. And the point α_3 is equidistant from the previous two. Rules are

provided for the automatic updating of the interval of interpolation.

In order to avoid numerical instabilities, a switching parameter is introduced in both the cubic interpolation prccess and the proposed alternative. This parameter depends on the relative magnitude and the signs of the coefficients appearing in the polynomial approximations to $f(\alpha)$ and $f_\alpha(\alpha)$. It governs the switch from the cubic to the quadratic approximation for $f(\alpha)$ and the switch from the quadratic to the linear approximation for $f_\alpha(\alpha)$. For an alternative switching parameter, see Ref. 9.

2. Review of Cubic Interpolation

Consider a unimodal function

$$f = f(\alpha) \quad , \tag{1}$$

where α is a scalar. Assume that the minimum of the function occurs for some value α_o which is finite and positive.[5] Next, consider the reference stepsize α_* and the sequence of stepsizes

$$\{a\} = \{0, \alpha_*, 2\alpha_*, 4\alpha_*, 8\alpha_*, \ldots\} \quad . \tag{2}$$

For every element of the sequence (2), compute the ordinate $f(\alpha)$ and the slope $f_\alpha(\alpha)$. Denote by α_1 and α_2 the smallest consecutive elements of the sequence (2) such that the following inequalities are satisfied:

$$f_\alpha(\alpha_1) < 0 \quad , \quad f_\alpha(\alpha_2) > 0 \quad . \tag{3}$$

Then, assuming that the derivative $f_\alpha(\alpha)$ is continuous, the minimum of $f(\alpha)$ occurs for a value α_o such that

$$\alpha_1 < \alpha_o < \alpha_2 \quad . \tag{4}$$

In order to find the minimum of $f(\alpha)$ numerically,

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[5] For simplicity, we assume that $f_\alpha(0) < 0$.

we represent the function $f(\alpha)$ in the cubic form

$$F(\alpha) = k_0 + k_1\alpha + k_2\alpha^2 + k_3\alpha^3 \quad . \tag{5}$$

The coefficients k_i are computed by forcing the cubic $F(\alpha)$ and its derivative $F_\alpha(\alpha)$ to satisfy the exact values of the ordinate $f(\alpha)$ and the slope $f_\alpha(\alpha)$ at α_1 and α_2 ; that is, the coefficients k_i are computed from the conditions

$$F(\alpha_1) = f(\alpha_1) \quad , \quad F_\alpha(\alpha_1) = f_\alpha(\alpha_1) \quad , \tag{6}$$

$$F(\alpha_2) = f(\alpha_2) \quad , \quad F_\alpha(\alpha_2) = f_\alpha(\alpha_2) \quad . \tag{7}$$

With the coefficients known, an approximation to the optimum stepsize α_o is obtained by determining the zero of the first derivative of (5), subject to the convexity condition for the cubic representation (5), that is,

$$F_\alpha(\alpha_o) = 0 \quad , \quad F_{\alpha\alpha}(\alpha_o) > 0 \quad . \tag{8}$$

Equation (8-1), in combination with Ineq. (8-2) and Eqs. (5)-(7), implies that (Ref. 10)

$$\alpha_o = \alpha_1 + \beta_o(\alpha_2 - \alpha_1) \quad , \tag{9}$$

where

$$\beta_o = (1/3c_3)[-c_2+\sqrt{(c_2^2-3c_1c_3)}] \quad , \quad \text{if } \rho \geq \varepsilon_2 \text{ or } c_2 \leq 0 \; ; \tag{10-1}$$

$$\beta_o = -c_1/2c_2 \quad , \quad \text{if } \rho < \varepsilon_2 \text{ and } c_2 > 0 \; . \tag{10-2}$$

In Eqs. (10), the coefficients c_1, c_2, c_3 are given by

$$c_1 = (\alpha_2-\alpha_1)\; f_\alpha(\alpha_1) \quad , \tag{11-1}$$

$$c_2 = 3[f(\alpha_2)-f(\alpha_1)]-(\alpha_2-\alpha_1)[2f_\alpha(\alpha_1)+f_\alpha(\alpha_2)] \quad , \tag{11-2}$$

$$c_3 = 2[f(\alpha_1)-f(\alpha_2)]+(\alpha_2-\alpha_1)[f_\alpha(\alpha_1)+f_\alpha(\alpha_2)] \quad , \tag{11-3}$$

and the switching parameter ρ is given by [6]

$$\rho = |\; 3c_1c_3/c_2^2 \;| \quad . \tag{12}$$

Use of (10-2) in place of (10-1) corresponds to setting $k_3=0$ in Eq. (5); that is, it corresponds to replacing the cubic approximation $F(\alpha)$ with a quadratic approximation. For the details, see Ref. 10.

Iterative Procedure. At the end of any iteration, an

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[6] An alternative switching parameter is presented by Acton in Ref. 9.

approximate optimum stepsize is known. Then, two possibilities arise, depending on the sign of $f_\alpha(\alpha)$ at the point α_o:

$$\text{Case (i)}\ , \qquad f_\alpha(\alpha_o) > 0 \ ; \tag{13-1}$$

$$\text{Case (ii)}\ , \qquad f_\alpha(\alpha_o) < 0 \ . \tag{13-2}$$

If the tilde denotes quantities pertaining to the next iteration, the resetting of α_1 and α_2 is done as follows:

$$\text{Case (i)}\ , \qquad \tilde{\alpha}_1 = \alpha_1\ , \quad \tilde{\alpha}_2 = \alpha_o \ ; \tag{14-1}$$

$$\text{Case (ii)}\ , \qquad \tilde{\alpha}_1 = \alpha_o\ , \quad \tilde{\alpha}_2 = \alpha_2 \ . \tag{14-2}$$

The iterative process is terminated whenever the optimum stepsize α_o satisfies the inequality

$$|\ f_\alpha(\alpha_o)\ | \leq \varepsilon_1 \ , \tag{15}$$

where ε_1 is a small, positive number.

Concerning function evaluations, the conclusions are as follows. For the first iteration, one needs to evaluate two functions and two derivatives. For subsequent iterations, one needs to evaluate only one additional function and one additional derivative, since the values of the function and its derivative at the endpoints of the previous interval are known and stored.

3. Modifications of the Cubic Interpolation Process

Generally speaking, the cubic interpolation process described in Section 2 enables one to find the minimum of a unimodal function in a relatively small number of iterations. However, it is known that pathological cases can be constructed such that this process might become slow and inefficient: for some extremely flat bowl functions (see Examples 5.21 and 5.22), the previous algorithm might be unable to converge in several hundred iterations.

In an effort to bypass the above difficulty, we present here two modifications of the previous process. The basic idea is to force a substantial reduction of the interval of interpolation through a bisection procedure, which can be either nonoptional [Modification M1] or optional [Modification M2].

We emphasize that, in the modifications described below, Eqs. (9)-(12) are retained. However, the updating formulas (13)-(14) are discarded and are replaced by new updating formulas, designed to force a more drastic reduction in the interval of interpolation.

Modification M1. Suppose that Eqs. (9)-(12) are employed in any given iteration. Also, suppose that, prior to starting the next iteration, the interval of interpolation associated with the procedure of Section 2 is bisected through

the consideration of the following intermediate stepsize:

$$\alpha_3 = (\alpha_1+\alpha_o)/2 \quad , \quad \text{if} \quad f_\alpha(\alpha_o) > 0 \quad ; \qquad (16\text{-}1)$$

$$\alpha_3 = (\alpha_o+\alpha_2)/2 \quad , \quad \text{if} \quad f_\alpha(\alpha_o) < 0 \quad . \qquad (16\text{-}2)$$

Then, four possibilites arise, depending on the signs of the slope $f_\alpha(\alpha)$ at α_o and α_3:

$$\text{Case (i)} \quad , \quad f_\alpha(\alpha_o) > 0 \quad , \quad f_\alpha(\alpha_3) > 0 \quad ; \qquad (17\text{-}1)$$

$$\text{Case (ii)} \quad , \quad f_\alpha(\alpha_o) > 0 \quad , \quad f_\alpha(\alpha_3) < 0 \quad ; \qquad (17\text{-}2)$$

$$\text{Case (iii)}, \quad f_\alpha(\alpha_o) < 0 \quad , \quad f_\alpha(\alpha_3) > 0 \quad ; \qquad (17\text{-}3)$$

$$\text{Case (iv)} \quad , \quad f_\alpha(\alpha_o) < 0 \quad , \quad f_\alpha(\alpha_3) < 0 \quad . \qquad (17\text{-}4)$$

If the tilde denotes quantities pertaining to the next iteration, the resetting of α_1 and α_2 is done as follows:

$$\text{Case (i)} \quad , \quad \tilde{\alpha}_1 = \alpha_1 \quad , \quad \tilde{\alpha}_2 = \alpha_3 \quad ; \qquad (18\text{-}1)$$

$$\text{Case (ii)} \quad , \quad \tilde{\alpha}_1 = \alpha_3 \quad , \quad \tilde{\alpha}_2 = \alpha_o \quad ; \qquad (18\text{-}2)$$

$$\text{Case (iii)}, \quad \tilde{\alpha}_1 = \alpha_o \quad , \quad \tilde{\alpha}_2 = \alpha_3 \quad ; \qquad (18\text{-}3)$$

$$\text{Case (iv)}\ , \quad \tilde{\alpha}_1 = \alpha_3 \ , \quad \tilde{\alpha}_2 = \alpha_2 \ . \tag{18-4}$$

It can be shown that any two consecutive intervals of interpolation satisfy the inequality

$$(\tilde{\alpha}_2 - \tilde{\alpha}_1) < (\alpha_2 - \alpha_1)/2 \ . \tag{19}$$

Consequently, Modification M1 should behave in a reasonable way, even in the pathological cases described previously. Of course, the iterative procedure is terminated whenever Ineq. (15) is satisfied.

Concerning function evaluations, the conclusions are as follows. For the first iteration, one needs to evaluate two functions and two derivatives. For subsequent iterations, one needs to evaluate two additional functions and two additional derivatives. Therefore, while Modification M1 is more robust than the standard cubic interpolation process of Section 2, a price must be paid in terms of function evaluations.

Modification M2. This modification has characteristics which are intermediate between those of the standard cubic interpolation process and those of Modification M1. It constitutes an attempt to retain the robustness characteristics of Modification M1, while trying to reduce the total number of function evaluations and derivative evaluations.

Basic to Modification M2 is the consideration of two consecutive optimum stepsizes $\hat{\alpha}_o$ and α_o. Depending on the signs of the slope $f_\alpha(\alpha)$ at $\hat{\alpha}_o$ and α_o, two cases are possible:

$$\text{Case (a)}, \quad f_\alpha(\hat{\alpha}_o) f_\alpha(\alpha_o) < 0 \; ; \tag{20-1}$$

$$\text{Case (b)}, \quad f_\alpha(\hat{\alpha}_o) f_\alpha(\alpha_o) > 0 \; . \tag{20-2}$$

For each of these cases, the next interval of interpolation is determined as follows:

Case (a) , use updating rules (13)-(14) ; (21-1)

Case (b) , use updating rules (17)-(18) . (21-2)

The significance of the strategy described by (20)-(21) is as follows. For Case (a), (20-1) indicates that the signs of $f_\alpha(\hat{\alpha}_o)$ and $f_\alpha(\alpha_o)$ are different, meaning that the actual optimal stepsize lies inside the interval enclosed by $\hat{\alpha}_o$ and α_o; therefore, bisection is not applied. For Case (b), (20-2) indicates that the signs of $f_\alpha(\hat{\alpha}_o)$ and $f_\alpha(\alpha_o)$ are the same, meaning that actual optimal stepsize lies outside the interval enclosed by $\hat{\alpha}_o$ and α_o; therefore, bisection is applied.

In essence, Modification M2 proceeds as follows: For

Case (a), we employ the cubic interpolation process in its standard form; while, for Case (b), we employ Modification M1.

4. Alternatives to the Cubic Interpolation Process

An alternative to the cubic interpolation process is a Lagrange interpolation scheme: instead of employing the values of $f(\alpha)$ and $f_\alpha(\alpha)$ at two points, we employ the values of $f_\alpha(\alpha)$ at three points.

The computational procedure is as follows. We consider the sequence of stepsizes (2) and, for every element of the sequence, we compute the derivative $f_\alpha(\alpha)$. We denote by α_1 and α_2 the smallest consecutive elements of the sequence (2) such that Ineqs. (3) are satisfied. Next, we denote by

$$\alpha_3 = (\alpha_1+\alpha_2)/2 \tag{22}$$

the point equidistant from the previous two and, at this point, we compute the slope $f_\alpha(\alpha_3)$.

In order to find the minimum of $f(\alpha)$ numerically, we represent the derivative $f_\alpha(\alpha)$ in the quadratic form

$$F_\alpha(\alpha) = p_1+p_2\alpha+p_3\alpha^2 \quad . \tag{23}$$

The coefficients p_i are computed by forcing the quadratic (23) to satisfy the exact values of the slope $f_\alpha(\alpha)$ at α_1, α_2, α_3; that is, the coefficients p_i are computed from

the conditions

$$F_\alpha(\alpha_1) = f_\alpha(\alpha_1) , \quad F_\alpha(\alpha_2) = f_\alpha(\alpha_2) , \quad F_\alpha(\alpha_3) = f_\alpha(\alpha_3) , \tag{24}$$

which represent a Lagrange interpolation scheme with equidistant arguments.

With the coefficients known, an approximation to the optimum stepsize is obtained by determining the zero of $F_\alpha(\alpha)$, subject to the positiveness condition for $F_{\alpha\alpha}(\alpha)$. Equation (8-1), in combination with Ineq. (8-2) and Eqs. (23)-(24), implies that (Ref. 10)

$$\alpha_o = (\alpha_1+\alpha_2)/2 + \gamma_o(\alpha_2-\alpha_1)/2 , \tag{25}$$

where

$$\gamma_o = (1/2q_3)[-q_2 + \sqrt{(q_2^2-4q_1q_3)}] , \text{ if } \sigma \geq \varepsilon_2 ; \tag{26-1}$$

$$\gamma_o = -q_1/q_2 , \qquad \text{if } \sigma < \varepsilon_2 . \tag{26-2}$$

In Eqs. (26), the coefficients q_1, q_2, q_3 are given by

$$q_1 = f_\alpha(\alpha_3) , \tag{27-1}$$

$$q_2 = [f_\alpha(\alpha_2) - f_\alpha(\alpha_1)]/2 \quad , \tag{27-2}$$

$$q_3 = -f_\alpha(\alpha_3) + [f_\alpha(\alpha_1) + f_\alpha(\alpha_2)]/2 \quad , \tag{27-3}$$

and the switching parameter σ is given by

$$\sigma = |\ 4q_1q_3/q_2^2\ | \quad . \tag{28}$$

Use of (26-2) in place of (26-1) corresponds to setting $p_3=0$ in Eq. (23); that is, it corresponds to replacing the quadratic approximation to the derivative $f_\alpha(\alpha)$ with a linear approximation. For the details, see Ref. 10.

Version A1. In this version, two possibilities arise, depending on the sign of $f_\alpha(\alpha)$ at the point α_o :

$$\text{Case (i),} \quad f_\alpha(\alpha_o) > 0 \quad ; \tag{29-1}$$

$$\text{Case (ii),} \quad f_\alpha(\alpha_o) < 0 \quad . \tag{29-2}$$

The resetting of α_1 and α_2 is done as follows:

$$\text{Case (i),} \quad \tilde{\alpha}_1 = \alpha_1 \quad , \quad \tilde{\alpha}_2 = \alpha_o \quad ; \tag{30-1}$$

$$\text{Case (ii),} \quad \tilde{\alpha}_1 = \alpha_o \quad , \quad \tilde{\alpha}_2 = \alpha_2 \quad . \tag{30-2}$$

The iterative process is terminated whenever the optimum step-size α_o satisfies Ineq. (15).

Concerning function evaluations, the conclusions are as follows. For the first iteration, one needs to evaluate three derivatives. For subsequent iterations, one needs to evaluate two additional derivatives, since the values of the derivatives at the endpoints of the previous interval are known and stored.

<u>Version A2</u>. In this version, four possibilities arise, depending on the signs of $f_\alpha(\alpha)$ at points α_3 and α_o :

$$\text{Case (i)}, \quad f_\alpha(\alpha_3) > 0 \;, \quad f_\alpha(\alpha_o) > 0 \;; \tag{31-1}$$

$$\text{Case (ii)}, \quad f_\alpha(\alpha_3) > 0 \;, \quad f_\alpha(\alpha_o) < 0 \;; \tag{31-2}$$

$$\text{Case (iii)}, \quad f_\alpha(\alpha_3) < 0 \;, \quad f_\alpha(\alpha_o) > 0 \;; \tag{31-3}$$

$$\text{Case (iv)}, \quad f_\alpha(\alpha_3) < 0 \;, \quad f_\alpha(\alpha_o) < 0 \;. \tag{31-4}$$

The resetting of α_1 and α_2 is done as follows:

$$\text{Case (i)}, \quad \tilde{\alpha}_1 = \alpha_1 \;, \quad \tilde{\alpha}_2 = \alpha_o \;; \tag{32-1}$$

$$\text{Case (ii)}, \quad \tilde{\alpha}_1 = \alpha_o \;, \quad \tilde{\alpha}_2 = \alpha_3 \;; \tag{32-2}$$

$$\text{Case (iii)}, \quad \tilde{\alpha}_1 = \alpha_3 \ , \quad \tilde{\alpha}_2 = \alpha_o \ ; \tag{32-3}$$

$$\text{Case (iv)}, \quad \tilde{\alpha}_1 = \alpha_o \ , \quad \tilde{\alpha}_2 = \alpha_2 \ . \tag{32-4}$$

The iterative process is terminated whenever the optimum step-size α_o satisfies Ineq. (15).

Concerning function evaluations, the conclusions are as follows. For the first iteration, one needs to evaluate three derivatives. For subsequent iterations, one needs to evaluate two additional derivatives, since the values of the derivatives at the endpoints and the middlepoint of the previous interval are known and stored.

Remark. Concerning the reduction of the interval of interpolation, Version A1 does not have any particular property. On the other hand, Version A2 is such that any two consecutive intervals of interpolation satisfy the inequality

$$(\tilde{\alpha}_2 - \tilde{\alpha}_1) < (\alpha_2 - \alpha_1)/2 \ . \tag{33}$$

5. Experimental Conditions and Numerical Examples

In order to evaluate and compare the previous algorithms, twenty-nine numerical examples were solved. The algorithms were programmed in FORTRAN IV, and the numerical results were obtained using the IBM 370/155 computer of Rice University and double-precision arithmetic.

For all of the examples, the reference stepsize

$$\alpha_* = 1 \tag{34}$$

was employed, that is, the sequence of stepsizes explored was chosen as follows:

$$\{\alpha\} = \{0, 1, 2, 4, 8, \ldots\} \quad . \tag{35}$$

The algorithms were programmed to stop whenever Ineq. (15) was satisfied with

$$\varepsilon_1 = 10^{-5} \quad \text{or} \quad \varepsilon_1 = 10^{-10} \quad . \tag{36}$$

The switching constant ε_2 appearing in (10) and (26) was set at the level

$$\varepsilon_2 = 10^{-10} \quad . \tag{37}$$

The twenty-nine functions investigated[7] are described by Eqs. (38)-(66). For these functions, Table 1 supplies the abscissa of the minimal point α_o , the value of the function at the minimal point $f(\alpha_o)$, and the value of the second derivative at the minimal point $f_{\alpha\alpha}(\alpha_o)$. Of course, at the minimal point, one has $f_\alpha(\alpha_o) = 0$ within the degree of precision established by (36-2).

<u>Example 5.1</u>

$$f(\alpha) = (2\alpha-4.5)^4-75\alpha+295 \quad ; \tag{38}$$

<u>Example 5.2</u>

$$f(\alpha) = \alpha^6/6-3\alpha \quad ; \tag{39}$$

<u>Example 5.3</u>

$$f(\alpha) = 6/(0.0005+\alpha)+15/(1.0005-\alpha) \quad ; \tag{40}$$

<u>Example 5.4</u>

$$f(\alpha) = [\exp(\alpha-\sqrt{\pi})-\alpha+\sqrt{\pi}-1]^4+(\alpha-\sqrt{\pi})^8+(\alpha-\sqrt{\pi})^2 \quad ; \tag{41}$$

<u>Example 5.5</u>

$$f(\alpha) = [\exp(\alpha-e^2)-\alpha+e^2-1]^4+(\alpha-e^2)^8+(\alpha-e^2)^2 \quad ; \tag{42}$$

<u>Example 5.6</u>

$$f(\alpha) = [\exp(\alpha-3)-\alpha+2]^4+(\alpha-3)^8+(\alpha-3)^2 \quad ; \tag{43}$$

<u>Example 5.7</u>

$$f(\alpha) = \exp[(\alpha-\pi)^2+10(\alpha-\pi)^4] \quad ; \tag{44}$$

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[7]The symbol e in Eq. (42) denotes the basis of natural logarithms.

Example 5.8

$$f(\alpha) = -10\cos^5\alpha-\alpha \quad ; \qquad (45)$$

Example 5.9

$$f(\alpha) = -100\cos^5\alpha-\alpha \quad ; \qquad (46)$$

Example 5.10

$$f(\alpha) = -1000\cos^5\alpha-\alpha \quad ; \qquad (47)$$

Example 5.11

$$f(\alpha) = -10\cos^4\alpha-\alpha \quad ; \qquad (48)$$

Example 5.12

$$f(\alpha) = -100\cos^4\alpha-\alpha \quad ; \qquad (49)$$

Example 5.13

$$f(\alpha) = -1000\cos^4\alpha-\alpha \quad ; \qquad (50)$$

Example 5.14

$$f(\alpha) = 100\cos\alpha-\alpha \quad ; \qquad (51)$$

Example 5.15

$$f(\alpha) = \cos^5(\alpha+\pi/6) \quad ; \qquad (52)$$

Example 5.16

$$f(\alpha) = \cos^9(\alpha+\pi/6) \quad ; \qquad (53)$$

Example 5.17

$$f(\alpha) = 500\cos^5(\alpha+\pi/6)-\alpha \quad ; \qquad (54)$$

Example 5.18

$$f(\alpha) = -\pi\alpha/4-\pi^2\alpha^2+100\sin^7(\pi\alpha/4) \quad ; \qquad (55)$$

Example 5.19

$$f(\alpha) = 1-\exp[-(\alpha-\pi)^2] \quad ; \qquad (56)$$

Example 5.20

$$f(\alpha) = 1-10\ \exp[-(\alpha-\pi)^2] \quad ; \tag{57}$$

Example 5.21

$$f(\alpha) = 1-\exp[-(2\alpha-\pi+2)^8] \quad ; \tag{58}$$

Example 5.22

$$f(\alpha) = 1-10\ \exp[-(2\alpha-\pi+2)^8] \quad ; \tag{59}$$

Example 5.23

$$f(\alpha) = 100-10\alpha+0.05\ \sinh(20\alpha) \quad ; \tag{60}$$

Example 5.24

$$f(\alpha) = 99-10\alpha+\cosh(20\alpha) \quad ; \tag{61}$$

Example 5.25

$$f(\alpha) = 100-10\alpha+0.05\alpha^4\sinh(20\alpha) \quad ; \tag{62}$$

Example 5.26

$$f(\alpha) = 99-10\alpha+\alpha^4\cosh(20\alpha) \quad ; \tag{63}$$

Example 5.27

$$f(\alpha) = 100-10000\alpha+0.05\alpha^4\sinh(20\alpha) \quad ; \tag{64}$$

Example 5.28

$$f(\alpha) = 100\ \cos(\sinh\ \alpha) \quad ; \tag{65}$$

Example 5.29

$$f(\alpha) = \cos[\exp(\alpha-1/3)] \quad . \tag{66}$$

Table 1. Solutions for the numerical examples.

Example	α_o	$f(\alpha_o)$	$f_{\alpha\alpha}(\alpha_o)$
5.1	0.3304 E+01	0.6694 E+02	0.2134 E+03
5.2	0.1245 E+01	-0.3114 E+01	0.1204 E+02
5.3	0.3873 E+00	0.3993 E+02	0.3358 E+03
5.4	0.1772 E+01	0.0000 E+00	0.2000 E+01
5.5	0.7389 E+01	0.0000 E+00	0.2000 E+01
5.6	0.3000 E+01	0.0000 E+00	0.2000 E+01
5.7	0.3141 E+01	0.1000 E+01	0.2000 E+01
5.8	0.2001 E-01	-0.1001 E+02	0.4986 E+02
5.9	0.2000 E-02	-0.1000 E+03	0.4999 E+03
5.10	0.2000 E-03	-0.1000 E+04	0.4999 E+04
5.11	0.2502 E-01	-0.1001 E+02	0.3987 E+02
5.12	0.2500 E-02	-0.1000 E+03	0.3999 E+03
5.13	0.2500 E-03	-0.1000 E+04	0.3999 E+04
5.14	0.3151 E+01	-0.1031 E+03	0.9999 E+02
5.15	0.2617 E+01	-0.1000 E+01	0.5000 E+01
5.16	0.2617 E+01	-0.1000 E+01	0.9000 E+01
5.17	0.2618 E+01	-0.5026 E+03	0.2499 E+04
5.18	0.7790 E+00	-0.4539 E+01	0.7989 E+02
5.19	0.3141 E+01	0.0000 E+00	0.2000 E+01
5.20	0.3141 E+01	-0.9000 E+01	0.2000 E+02
5.21	0.5707 E+00	0.0000 E+00	0.0000 E+00
5.22	0.5707 E+00	-0.9000 E+01	0.0000 E+00
5.23	0.1496 E+00	0.9900 E+02	0.1989 E+03
5.24	0.2406 E-01	0.9987 E+02	0.4472 E+03
5.25	0.3415 E+00	0.9689 E+02	0.3062 E+03
5.26	0.2487 E+00	0.9678 E+02	0.3428 E+03
5.27	0.5870 E+00	-0.5397 E+04	0.2638 E+06
5.28	0.1862 E+01	-0.1000 E+03	0.1086 E+04
5.29	0.1478 E+01	-0.1000 E+01	0.9869 E+01

6. Numerical Results, Discussion, and Conclusions

In this paper, the numerical solution of the problem of minimizing a unimodal function $f(\alpha)$ is considered, where α is a scalar. Two processes are studied. One is the cubic interpolation process, in which the coefficients of the cubic approximation to the function are determined from the values of the ordinate $f(\alpha)$ and the slope $f_\alpha(\alpha)$ at two points α_1 and α_2, chosen so that $f_\alpha(\alpha_1) < 0$ and $f_\alpha(\alpha_2) > 0$. The other is an alternative to the former process, in which the coefficients of the resulting quadratic approximation to the derivative of the function are determined from the values of the slope $f_\alpha(\alpha)$ at three points, namely, α_1, α_2, and $\alpha_3 = (\alpha_1+\alpha_2)/2$. Therefore, the cubic interpolation process is replaced by a Lagrange interpolation scheme based on three points with equidistant arguments.

The iterative procedure for the cubic interpolation process is investigated in three schemes: the standard process SP, Modification M1, and Modification M2. Modification M1 includes the nonoptional bisection of the interval of interpolation, and Modification M2 includes the optional bisection of the interval of interpolation, in accordance with the rules of Section 3.

The iterative procedure for the alternative process is investigated in two schemes: Version A1 and Version A2. Each

version involves different updating rules for the endpoints of the interval of interpolation, in accordance with the rules of Section 4.

The resulting algorithms are compared through 29 numerical examples. For these examples, Tables 2 and 3 show the number of iterations for convergence N to the stopping condition (36-1) or the stopping condition (36-2).

Comparison of Algorithms. Inspection of Tables 2 and 3 shows that the standard cubic interpolation process SP fails to converge in two examples (Examples 5.21 and 5.22), while the proposed modifications and alternatives converge in every case.

For the 27 examples where all of the algorithms converge, it is of interest to compute the cumulative number of iterations for convergence ΣN. This yields the data summarized in Table 4.

Starting from the above data, one can compute the average relative change in number of iterations for convergence, by comparison with Algorithm SP. This yields the data summarized in Table 5.

It becomes evident that Algorithms M1 and A2 are the best among those presented in this paper. However, one must remember that one iteration of Algorithm M1 or Algorithm A2 takes longer than one iteration of Algorithm SP. Therefore,

there is clearly a trade off between robustness and rapidity of convergence.

Detailed Behaviour of the Algorithms. For one particular example (namely, Example 5.29) and for the stopping condition (36-1), the detailed behavior of the five algorithms investigated is illustrated in Tables 6-10.

Supplementary Computations. After completion of this work, Examples 5.1 through 5.29 were rerun by replacing the stopping condition (15) with the stopping condition

$$| \alpha_o - \hat{\alpha}_o | \leq \varepsilon_1 \quad . \tag{67}$$

Here, α_o denotes the optimum stepsize associated with the present iteration, and $\hat{\alpha}_o$ denotes the optimum stepsize associated with the previous iteration. For these supplementary runs, results qualitatively consistent with those of Tables 2 and 3 were obtained, even though some slight changes were detected in the number of iterations for convergence.

Table 2. Number of iterations for convergence N, $\varepsilon_1 = 10^{-5}$.

Example	Algorithm				
	SP	M1	M2	A1	A2
5.1	4	4	4	4	4
5.2	4	3	4	4	4
5.3	6	4	5	5	5
5.4	3	2	3	3	3
5.5	5	4	4	5	5
5.6	4	3	3	1	1
5.7	7	4	7	6	6
5.8	2	2	2	4	4
5.9	2	2	2	5	4
5.10	2	3	2	5	4
5.11	5	4	5	6	4
5.12	5	4	5	6	5
5.13	5	4	5	6	5
5.14	7	4	5	7	3
5.15	5	5	4	5	4
5.16	4	5	4	6	3
5.17	6	6	5	6	4
5.18	4	3	3	4	4
5.19	6	4	5	7	3
5.20	7	5	6	8	3
5.21	>100	3	4	3	3
5.22	>100	4	4	4	4
5.23	7	5	6	6	6
5.24	7	5	6	7	7
5.25	6	5	7	7	7
5.26	8	5	5	5	5
5.27	7	5	6	7	7
5.28	5	3	4	5	4
5.29	15	4	5	12	2

Table 3. Number of iterations for convergence N, $\varepsilon_1=10^{-10}$.

Example	Algorithm				
	SP	M1	M2	A1	A2
5.1	5	4	5	5	5
5.2	5	4	5	4	4
5.3	6	5	6	6	6
5.4	4	3	4	3	3
5.5	6	4	5	5	5
5.6	4	4	4	1	1
5.7	8	6	8	7	7
5.8	4	3	4	7	6
5.9	3	3	3	9	6
5.10	4	6	6	9	6
5.11	9	6	7	11	6
5.12	10	6	7	12	6
5.13	10	6	7	12	6
5.14	11	6	6	11	5
5.15	7	7	6	7	5
5.16	7	7	6	10	4
5.17	8	8	7	8	6
5.18	6	4	4	4	4
5.19	12	6	7	13	4
5.20	13	6	7	14	5
5.21	>100	4	7	4	4
5.22	>100	4	7	4	4
5.23	8	6	7	7	7
5.24	8	6	6	7	7
5.25	7	6	7	8	8
5.26	8	6	6	6	6
5.27	7	11	7	8	8
5.28	8	5	5	8	5
5.29	28	5	6	25	3

Table 4. Cumulative number of iterations for convergence ΣN.

Stopping condition	Algorithm				
	SP	M1	M2	A1	A2
$\varepsilon_1 = 10^{-5}$	148	107	122	152	116
$\varepsilon_1 = 10^{-10}$	216	149	158	227	144

Table 5. Average relative change in number of iterations for convergence, by comparison with the standard process.

Stopping condition	Algorithm				
	SP	M1	M2	A1	A2
$\varepsilon_1 = 10^{-5}$	0.0%	-27.7%	-17.6%	+2.7%	-21.6%
$\varepsilon_1 = 10^{-10}$	0.0%	-31.0%	-26.8%	+5.1%	-33.3%

Table 6. Results for Example 5.29, $\varepsilon_1=10^{-5}$, Algorithm SP.

N	α	$f(\alpha)$	$f_\alpha(\alpha)$	$f_{\alpha\alpha}(\alpha)$
1	1.37834	-0.955878	-0.835299	6.89306
2	1.43827	-0.992500	-0.369056	8.67721
3	1.46150	-0.998668	-0.159416	9.37583
4	1.47107	-0.999760	-0.068276	9.66196
5	1.47510	-0.999957	-0.029141	9.78167
6	1.47680	-0.999992	-0.012420	9.83225
7	1.47753	-0.999999	-0.005290	9.85372
8	1.47783	-1.000000	-0.002253	9.86284
9	1.47797	-1.000000	-0.000959	9.86673
10	1.47802	-1.000000	-0.000408	9.86838
11	1.47805	-1.000000	-0.000174	9.86908
12	1.47806	-1.000000	-0.000074	9.86938
13	1.47806	-1.000000	-0.000032	9.86951
14	1.47806	-1.000000	-0.000013	9.86956
15	1.47806	-1.000000	-0.000006	9.86959

Table 7. Results for Example 5.29, $\varepsilon_1=10^{-5}$, Algorithm M1.

N	α	$f(\alpha)$	$f_\alpha(\alpha)$	$f_{\alpha\alpha}(\alpha)$
1	1.37834	-0.955878	-0.835299	6.89306
2	1.47608	-0.999980	-0.019521	9.81081
3	1.47805	-1.000000	-0.000120	9.86924
4	1.47806	-1.000000	-0.000000	9.86960

Table 8. Results for Example 5.29, $\varepsilon_1=10^{-5}$, Algorithm M2.

N	α	$f(\alpha)$	$f_\alpha(\alpha)$	$f_{\alpha\alpha}(\alpha)$
1	1.37834	-0.955878	-0.835299	6.89306
2	1.43827	-0.992500	-0.369056	8.67721
3	1.47606	-0.999980	-0.019664	9.81038
4	1.47805	-1.000000	-0.000174	9.86908
5	1.47806	-1.000000	-0.000000	9.86960

Table 9. Results for Example 5.29, $\varepsilon_1=10^{-5}$, Algorithm A1.

N	α	$f(\alpha)$	$f_\alpha(\alpha)$	$f_{\alpha\alpha}(\alpha)$
1	1.46319	-0.998925	-0.143476	9.42662
2	1.47206	-0.999823	-0.058742	9.69129
3	1.47562	-0.999971	-0.024046	9.79712
4	1.47706	-0.999995	-0.009843	9.84002
5	1.47765	-0.999999	-0.004029	9.85751
6	1.47790	-1.000000	-0.001649	9.86466
7	1.47799	-1.000000	-0.000675	9.86758
8	1.47804	-1.000000	-0.000276	9.86878
9	1.47805	-1.000000	-0.000113	9.86927
10	1.47806	-1.000000	-0.000046	9.86947
11	1.47806	-1.000000	-0.000019	9.86955
12	1.47806	-1.000000	-0.000008	9.86958

Table 10. Results for Example 5.29, $\varepsilon_1=10^{-5}$, Algorithm A2.

N	α	$f(\alpha)$	$f_\alpha(\alpha)$	$f_{\alpha\alpha}(\alpha)$
1	1.46319	-0.998925	-0.143476	9.42662
2	1.47806	-1.000000	-0.000006	9.86959

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